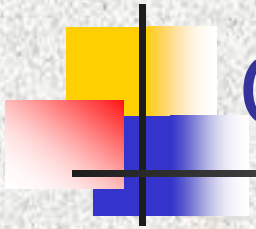
Multiscale Modeling of Crystaline Materials: The Quasicontinuum Method at Finite Temperature

L. Dupuy,
Division of Engineering and Applied science, California Institute of Technology, USA

In collaboration with:
R. Miller[1], E. Tadmor[2], R. Phillips[3]
[1]Department of Mechanical and Aerospace Engineering, Carleton University, Canada
[2]Faculty of Mechanical Engineering, Technion – Israel Institute of Technology, Israel
[3]Division of Engineering and Applied science, California Institute of Technology, USA



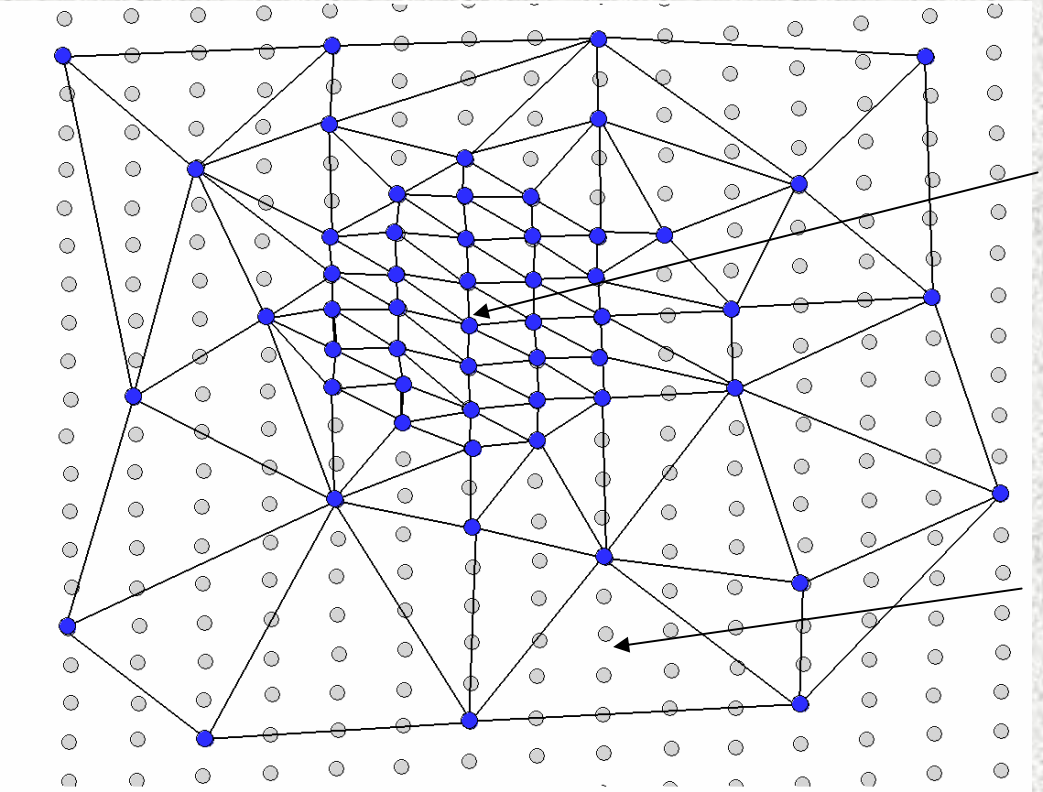
Outline

- 1. The Quasicontinuum method
- 2. Coarse-grained molecular dynamics
- 3. Implementation
- 4. Validation of the method
- 5. Nanoindentation simulations
- 6. Current issues and conclusion

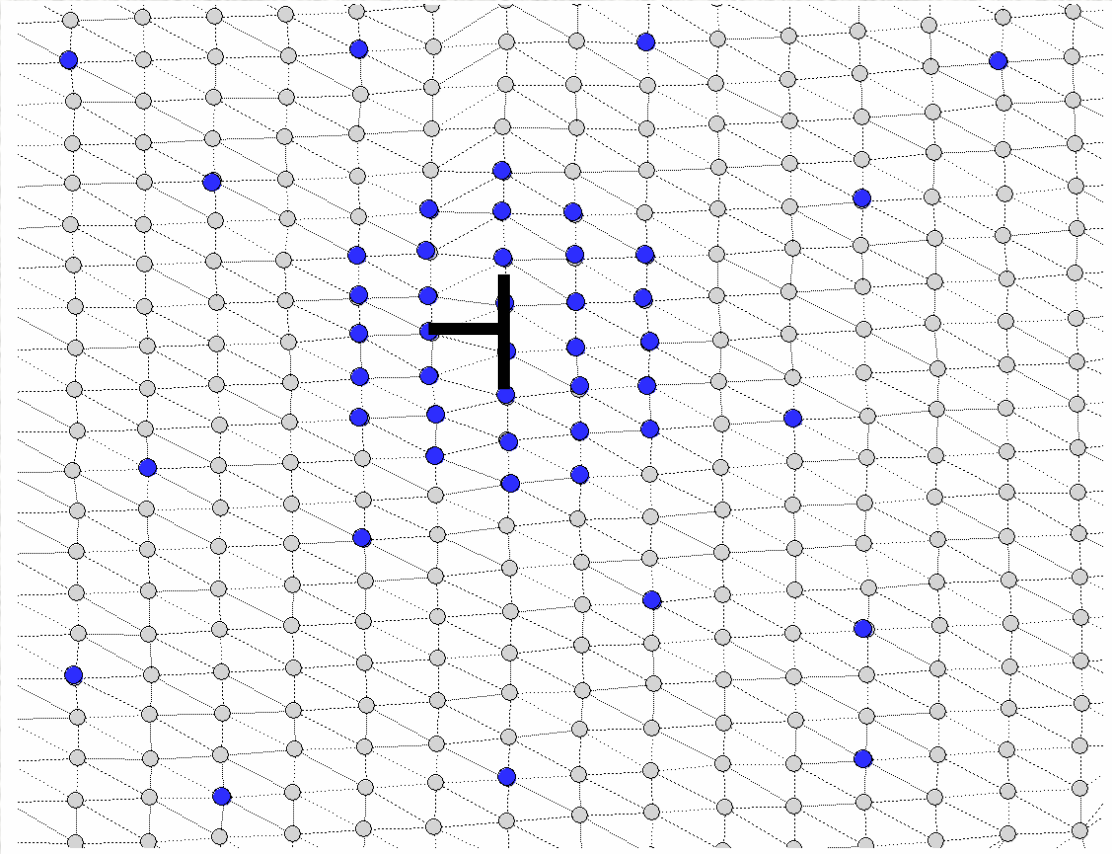
1. The Quasicontinuum method

(E. Tadmor, R. Miller, V. Shenoy, D. Rodney, R. Phillips, M. Ortiz)

- Implementation in the QC code: www.qcmethod.com
- Energy minimization technique at 0K with a reduced number of degrees of freedom



2. Coarse-grained MD



- Only a few atoms are involved in the critical mechanism

2. Coarse-grained MD: Requirements

- The coarse-grained system should behave like the full atomistic system:
  - Recover the equilibrium properties of the system at finite temperature as time averages over the trajectories:

$$\overline{A}\left(q_i^r\right)_{Coarse-grained} = \left\langle A\left(q_i^r\right)\right\rangle_{NVT}$$

  - The equations of motions in the atomistic regions should be as close as possible to the full system
  - The coarse-grained regions ensure the appropriate boundary conditions

2. Coarse grained MD: Potential energy

- Assumption: At each time step, the slave/missing atoms are at equilibrium

$$\hat{V}\left(q^r,\beta\right)=-\frac{1}{\beta}\ln\iiint_{slaves}\exp\left[-\beta V\left(q^r,q^s\right)\right]dq^s$$

- Restriction to problems close to equilibrium
- We need an approximation scheme to calculate the coarse-grained-potential energy

2. Coarse grained MD: Kinetic energy

- We use the lumped mass approach:

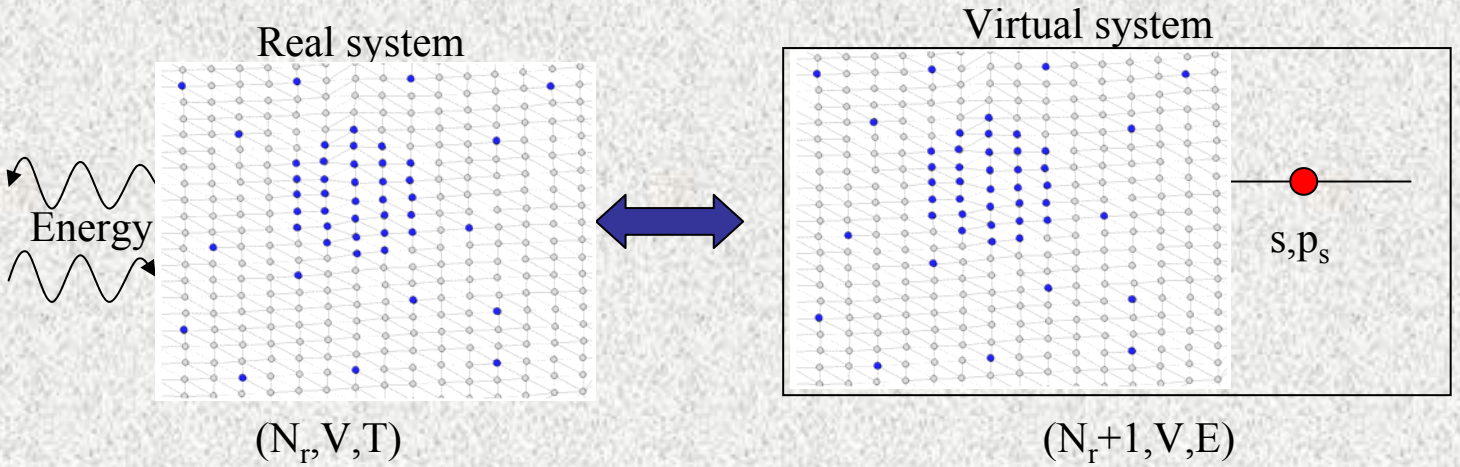
$$M_i^r = n_i m$$

- The coarse-grained potential energy can be written as:

$$\hat{E}_c\left(p^r\right) = \sum_{representative} \frac{\left(p_i^r\right)^2}{2M_i^r}$$

2. Coarse grained energy: Thermostat

- Nosé-Poincaré Thermostat



- Hamiltonian dynamics: the algorithm satisfies the symplectic condition
- Real time = Virtual time

2. Coarse grained MD: Dynamical behavior in the atomistic regions

- Equations of motion

$$\frac{dq_i^r}{dt} = \frac{p_i^r}{M_i^r} = \frac{p_i}{m_i}$$

$$\frac{dp_i^r}{dt} = -\frac{\partial \hat{V}}{\partial q_i^r}\left(q^r, \beta\right) - \frac{p_s}{Q} p_i^r = -\frac{\partial V}{\partial q_i}(q) - \frac{p_s}{Q} p_i$$

- Time-correlation functions

$$\left\langle p_i^r(t) p_i^r(0) \right\rangle = \frac{3M_i^r}{\beta} - \frac{3}{2\beta}\left\langle \frac{\partial^2 \hat{V}}{\partial q_i^{r\,2}}\left(q^r, \beta\right)\right\rangle_{NVT} t^2 - \frac{3M_i^r}{2Q\beta^2} t^2 + \theta\left(t^3\right)$$

$$\left\langle p_i^r(t) p_i^r(0) \right\rangle = \frac{3m_i}{\beta} - \frac{3}{2\beta}\left\langle \frac{\partial^2 V}{\partial q_i^2}(q)\right\rangle_{NVT} t^2 - \frac{3m_i}{2Q\beta^2} t^2 + \theta\left(t^3\right)$$

  - Choice of the mass of the thermostat

$$Q \approx \frac{N_r}{\beta \omega_E} \quad where \quad \omega_E = \sqrt{\frac{\partial^2 V}{\partial q^2}\Big/ m}$$

2. Coarse grained MD: Dynamical behavior in the coarse-grained regions

- Equations of motion

$$\frac{dq_i^r}{dt} = \frac{p_i^r}{M_i^r} \neq \frac{p_i}{m_i}$$

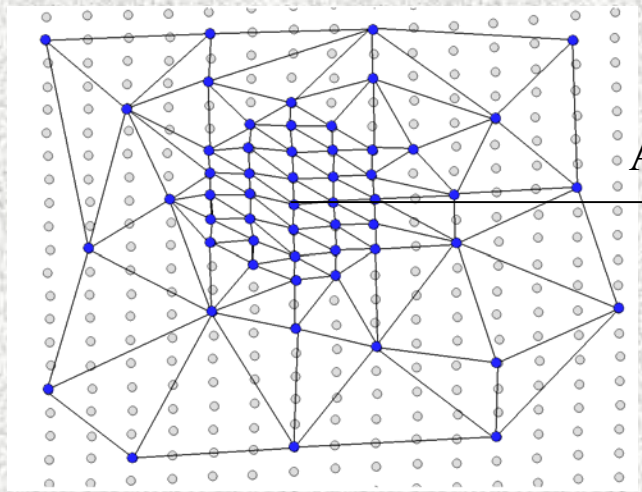
$$\frac{dp_i^r}{dt} = -\frac{\partial \hat{V}}{\partial q_i^r}\left(q^r, \beta\right) - \frac{p_s}{Q} p_i^r \neq -\frac{\partial V}{\partial q_i}(q) - \frac{p_s}{Q} p_i$$

- Time correlation functions

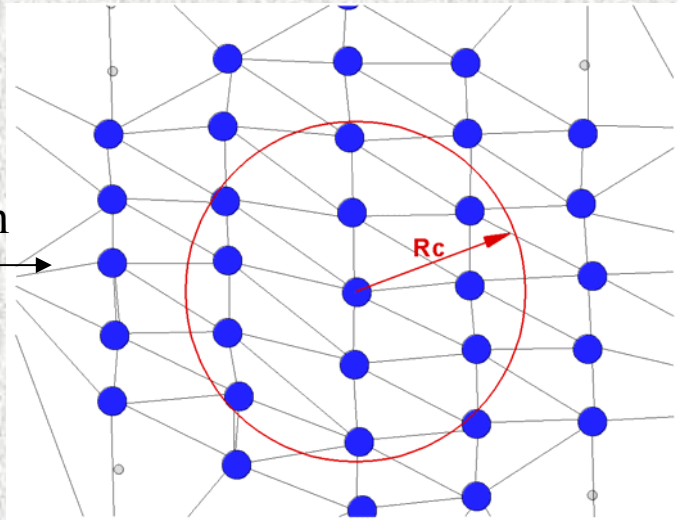
$$\left\langle p_i^r(t) p_i^r(0) \right\rangle = \frac{3M_i^r}{\beta} - \frac{3}{2\beta}\left\langle \frac{\partial^2 \hat{V}}{\partial {q_i^r}^2}\left(q^r, \beta\right)\right\rangle_{NVT} t^2 - \frac{3M_i^r}{2Q\beta^2} t^2 + \theta\left(t^3\right)$$

- The phonon spectrum is modified in the presence of coarse-grained regions

3. Implementation: Potential energy



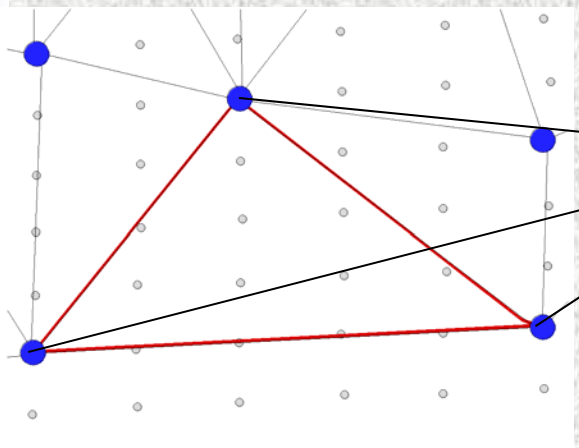
Atomistic region



$$\hat{V}(q^r,\beta) = -\frac{1}{\beta}\ln\iiint_{slave}\exp\left[-\beta U(q^r,q^s)\right]dq^s = \sum_{i\in atomistic} E_i^{at} - \frac{1}{\beta}\ln\iiint_{slave}\exp\left[-\beta U(q^r_{coarse},q^s)\right]dq^s$$

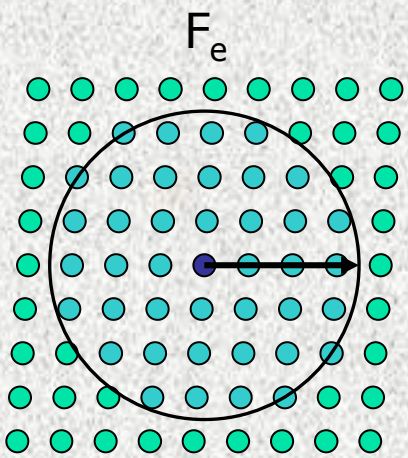
Exact

3. Implementation: Potential energy



- Deformation gradient F_e
- Cauchy-Born approximation

$$\hat{V}\left(q^r,\beta\right)\approx \sum_{i\in atomistic} E_i^{at} + \sum_{elements} \hat{E}_e\left(\underline{\underline{F}}_e,\beta\right)$$



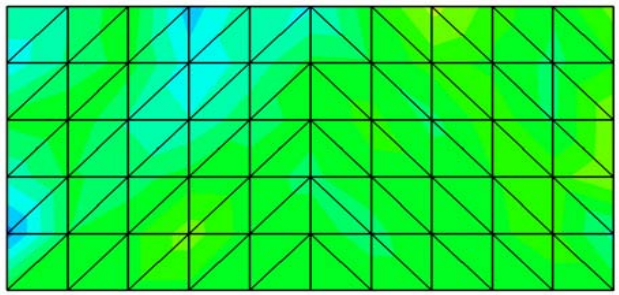
- Representative atoms: Energy $E^{at}\left(\underline{\underline{F}}_e\right)$
- Slave atoms: Free energy (Local Harmonic model – LeSar *et al.* 1989)

$$F^{at}\left(\underline{\underline{F}}_e,\beta\right)\approx E^{at}\left(\underline{\underline{F}}_e\right)+\frac{kT}{2}\ln\frac{\det \underline{\underline{D}}\left(\underline{\underline{F}}_e\right)}{\pi kT}$$

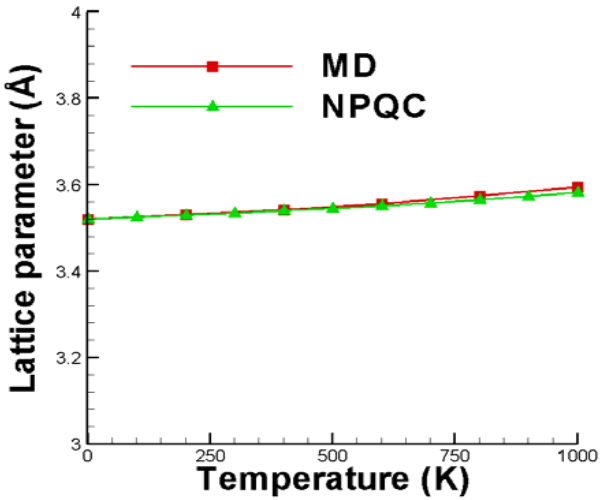
- Finally:

$$\hat{E}_e\left(\underline{\underline{F}}_e,\beta\right)\approx n_e^r E^{at}\left(\underline{\underline{F}}_e\right)+n_e^s F^{at}\left(\underline{\underline{F}}_e,\beta\right)$$

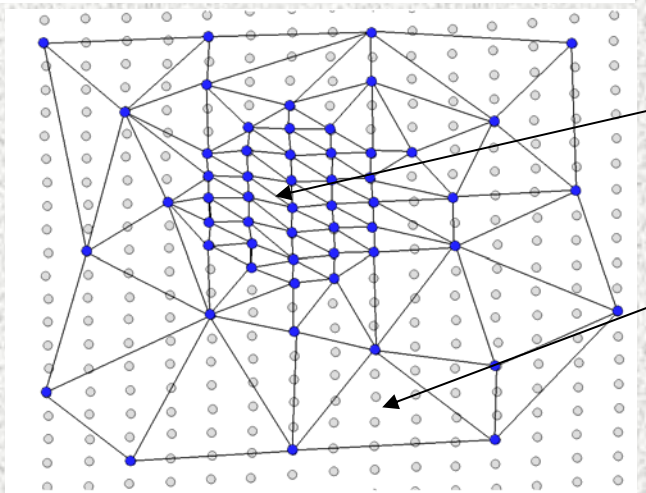
4. Validation: Thermal expansion



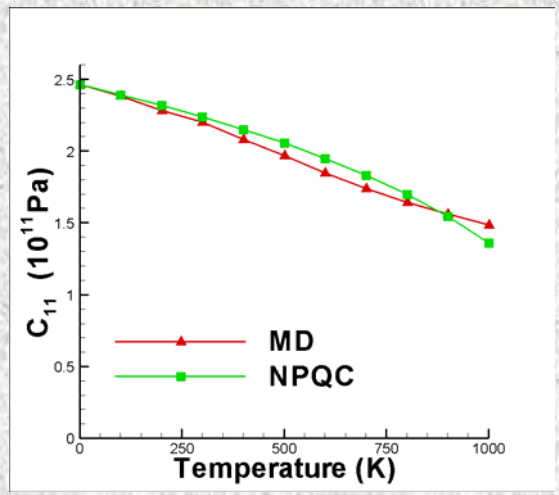
EAM Ni (Angelo 1995) - 200x100nm

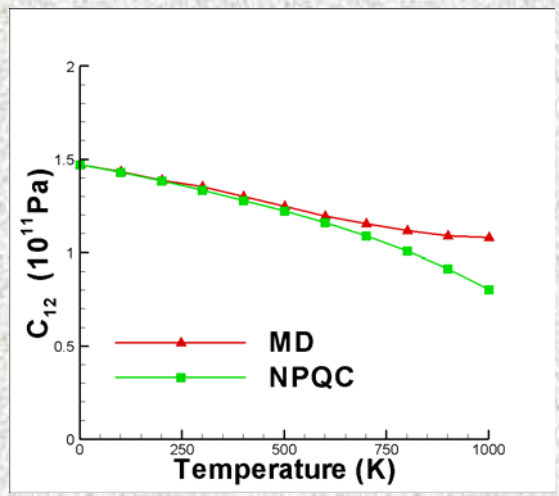


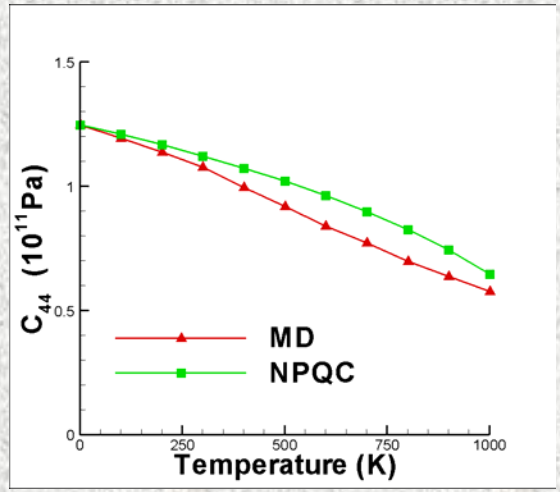
- Gold standard: MD
- Agreement within 0.3%
- Possible internal stress when combining atomistic and coarse-grained regions

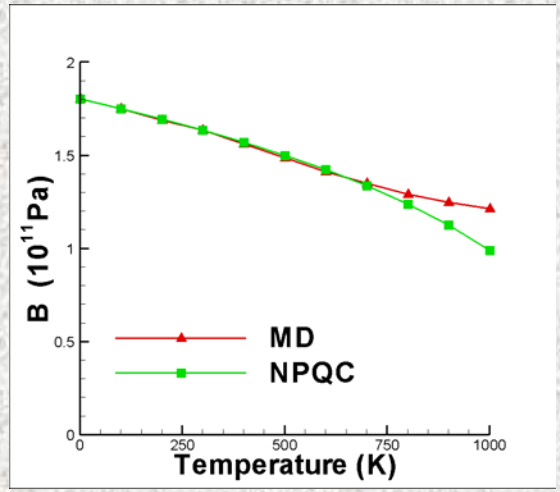


4. Validation: Elastic moduli



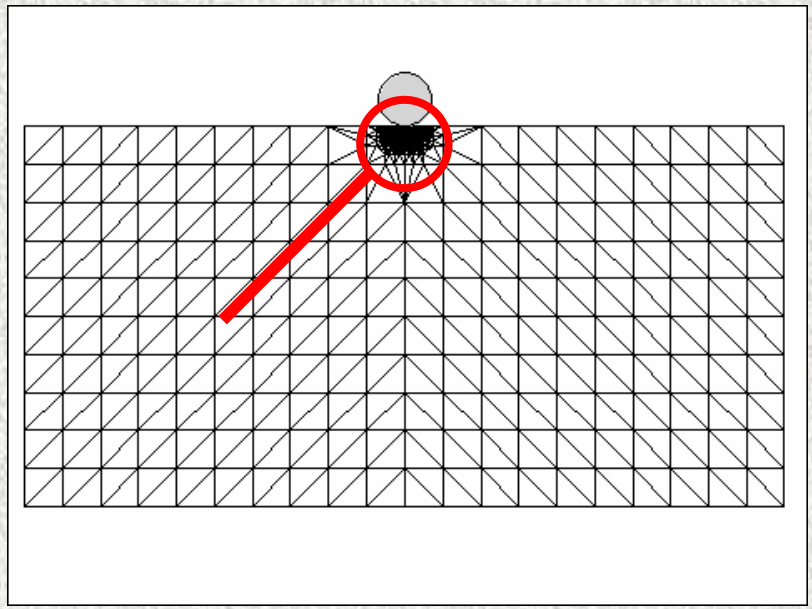






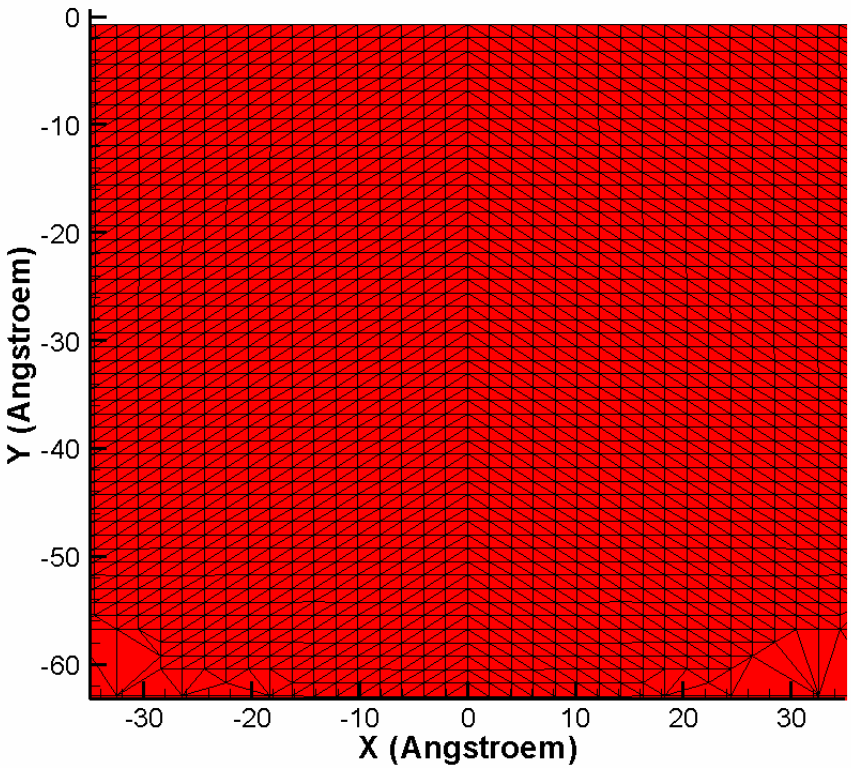
5. Nanoindentation simulations

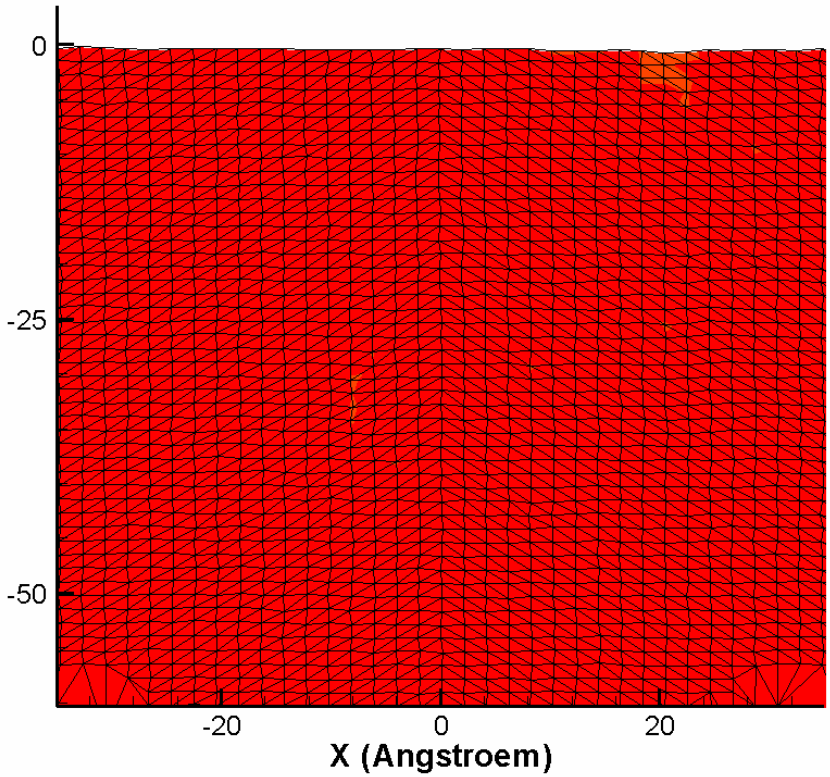
- Brinell indentation tests: R=70 Å
- Speed: 0.05Å/ps
- Sample: 2000x1000Å
- Equilibration time: 200 ps
- Total time: 600 ps
- Nickel – EAM Angelo (1995)



- 5000 representative atoms vs 10^7 atoms
- Speed up: ~ 10^3
- 24 hours on a regular computer (1GHz)

5. Nanoindentation simulations

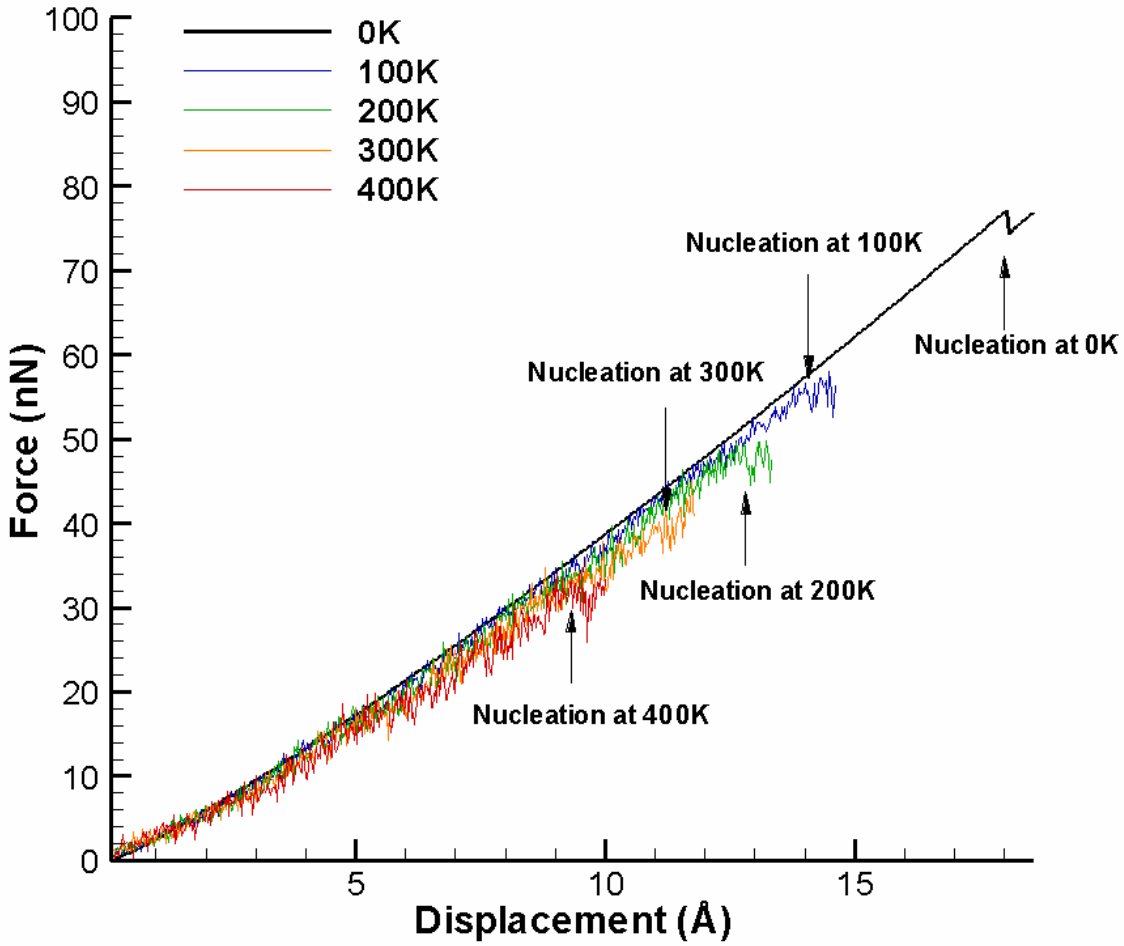


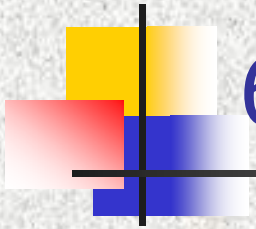


0K, quasi-static simulation

300K, NPQC simulation

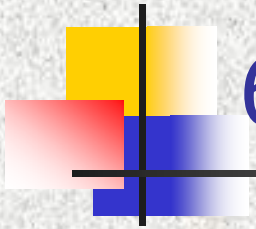
5. Nanoindentation simulations





6. Current issues

- Ghost forces:
  - Local/Non-local interface
    - Instabilities at higher temperature
  - Different equilibrium lattice parameters:
    - Can we do better at a reasonable computation cost?
- Wave reflection at the interface?
- Mesh adaption?



6. Conclusion

- Described the Nosé-Poincaré Quasicontinuum method. It allows to perform molecular dynamics without all the atoms at finite temperature.
- The equilibrium properties are recovered
- Application to nanoindentation simulations: Dislocation nucleation depends on temperature
- Next step: temperature dependence of fracture